Supporting Information

Role of Defects in Carbon Nanotube Walls in Deposition of CdS Nanoparticles from a Chemical Bath

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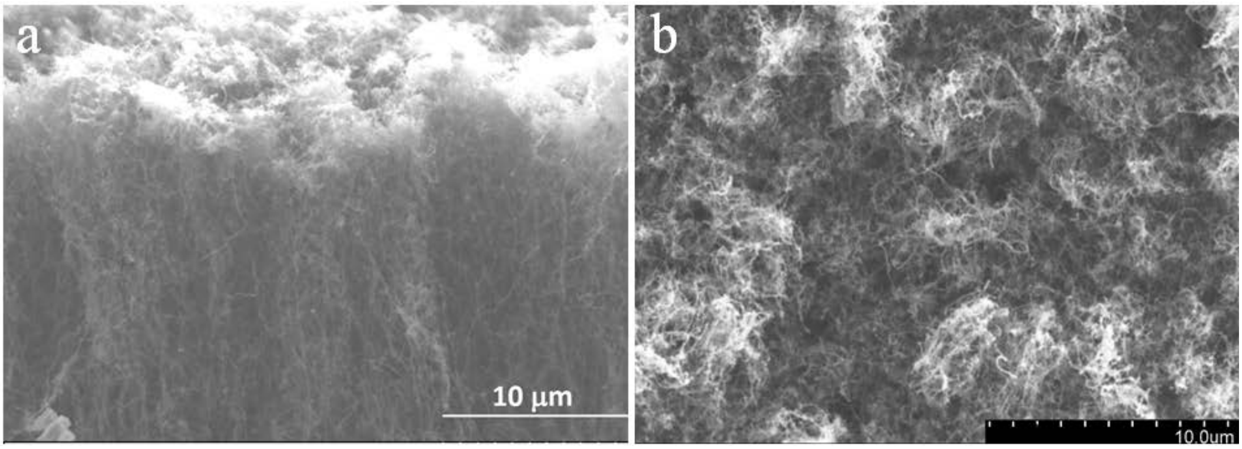

Figure S1. (a) – Scanning electron microscopy image of aligned MWCNT array with CdS nanoparticles deposited on the array top (light species). (b) – The image of top surface of the array. Deposition proceeded on the as-synthesized MWCNTs for 5 min. The images were obtained on a Hitachi S-3400N microscope.

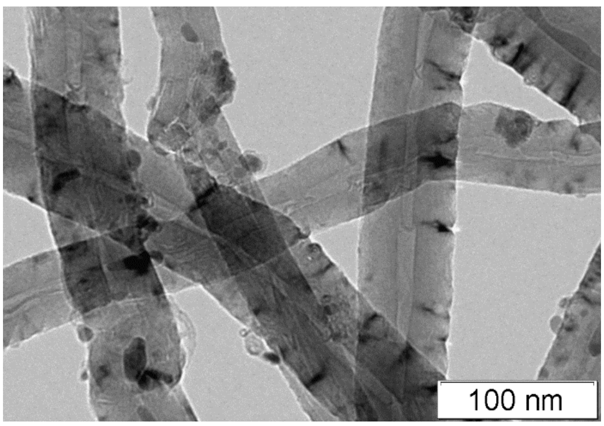

Figure S2. Low-magnification transmission electron microscopy image of multi-wall carbon nanotubes after deposition of CdS during 5 min. The image was obtained on a JEM 2010 microscope.

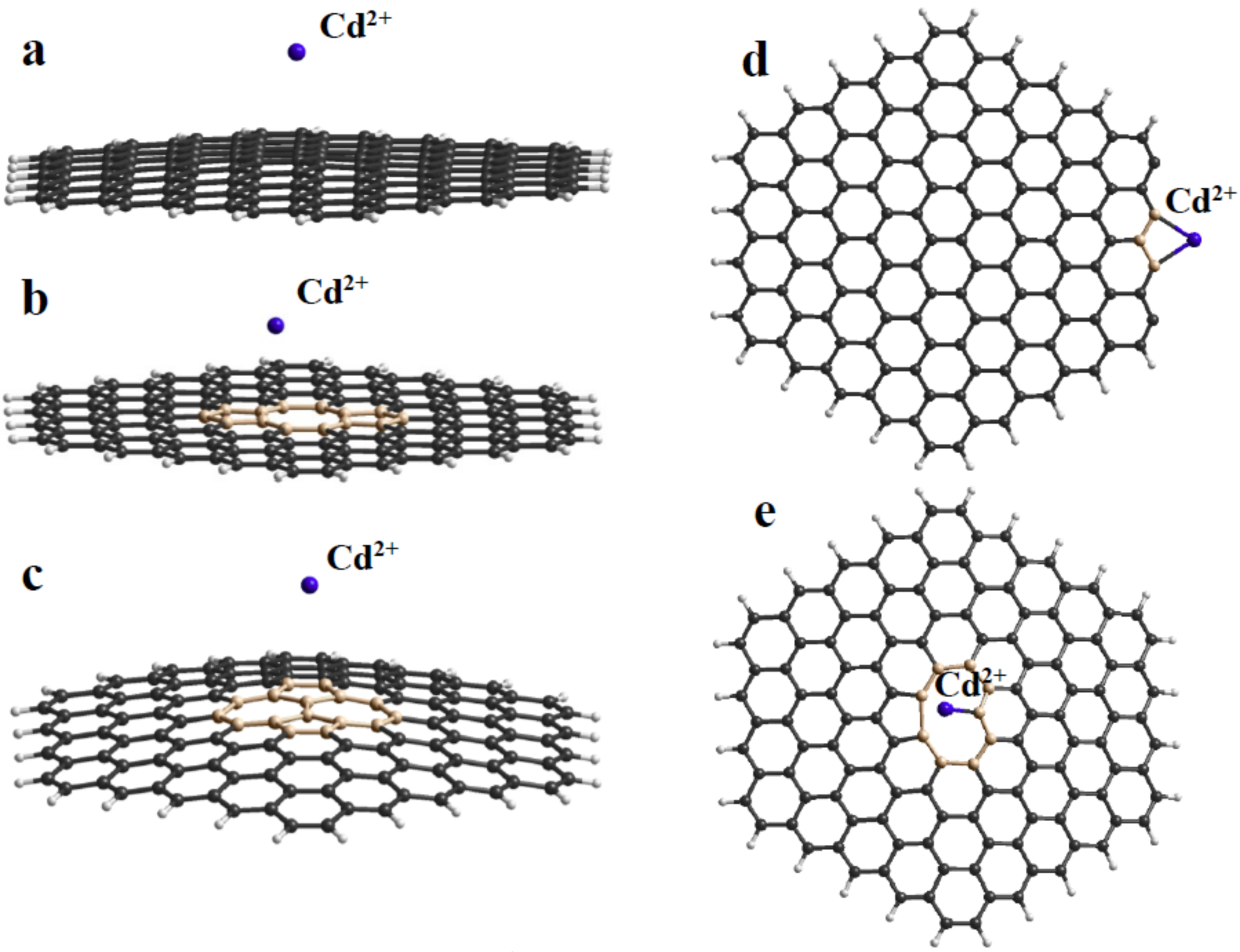

Figure S3. Graphene models with Cd^{2+} ion: (a) – perfect graphene fragment $C_{120}H_{28}$, (b) – fragment with a central divacancy defect, (c) – fragment with a central Stone-Wales defect, (d) fragment with a zigzag edge without terminating hydrogen atoms, (e) fragment with a central monovacancy defect. Carbon atoms constituting defects in graphene are highlighted. Geometry of the models was relaxed at the B3LYP/LACVP** level, for the models (a–c), optimization procedure was stopped when distance between Cd^{2+} and graphene exceeded 3.6 Å. As the result of relaxation, divacancy was reconstructed in 5–8–5 topological defect, monovacancy produced a pentagonal ring and *sp*-hybridized atom. Carbon atoms constituted defects are highlighted. The C–Cd length is ~2.29 Å in model (d) and ~2.27 Å in model (e).

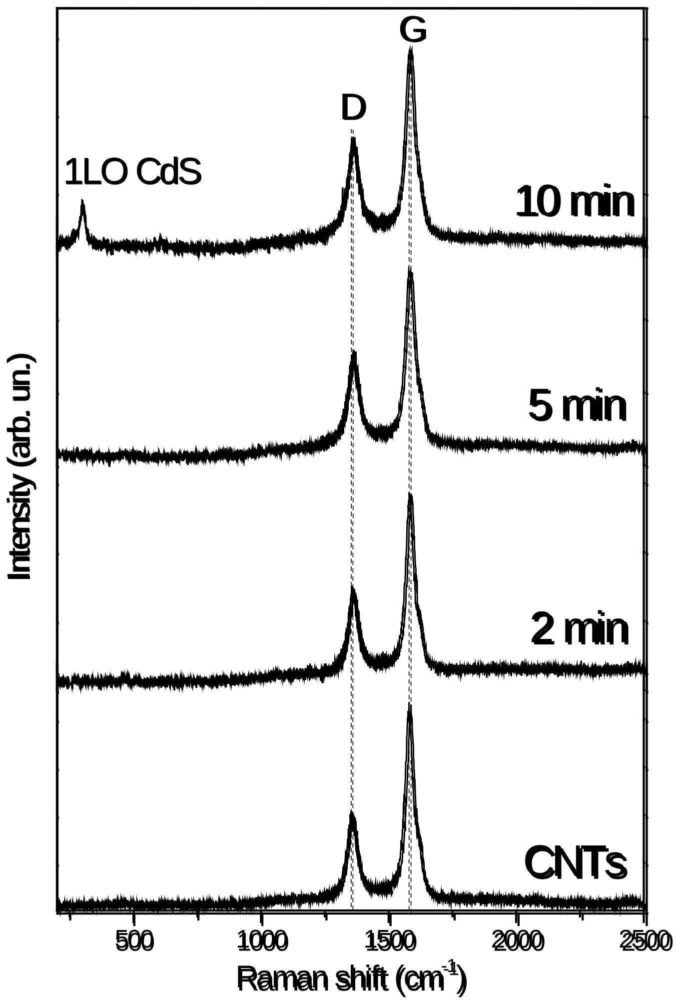

Figure S4. Raman spectra of the annealed MWCNTs before and after hosting in chemical bath for 2 min, 5 min, and 10 min. The spectrum of the last sample shows a peak corresponding to the 1LO band of CdS. The scattering was excited by 488 nm.

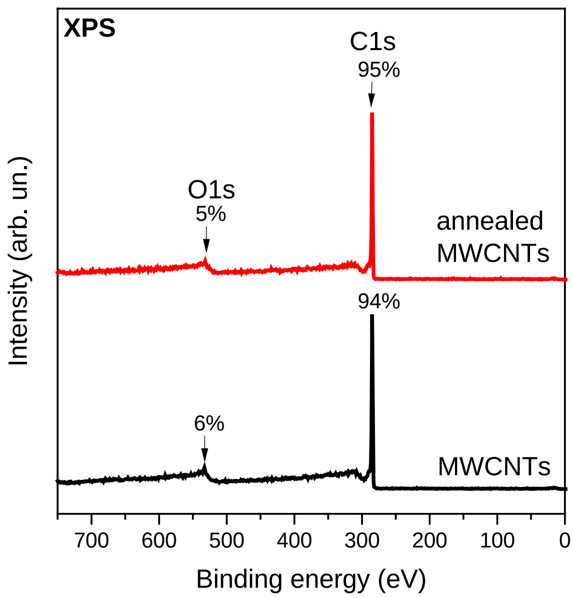

Figure S5. The overall XPS spectra measured at 800 eV for raw MWCNTs and MWCNTs annealed at 1000°C in a nitrogen flow for 2 h.

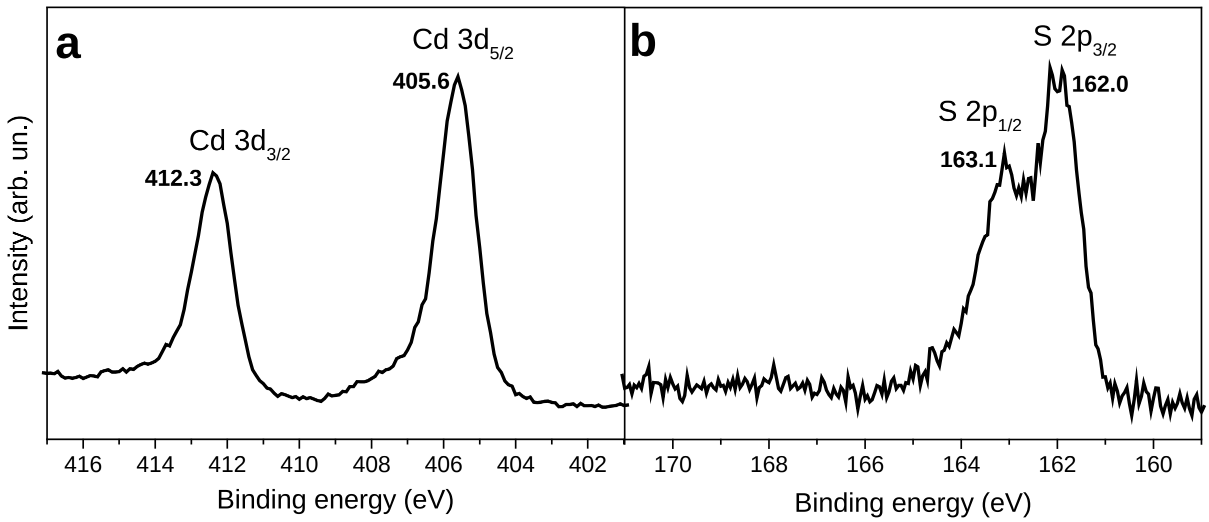

Figure S6. XPS Cd 3d (a) and S 2p (b) spectra of crystalline CdS measured at an excitation energy of 800 eV.

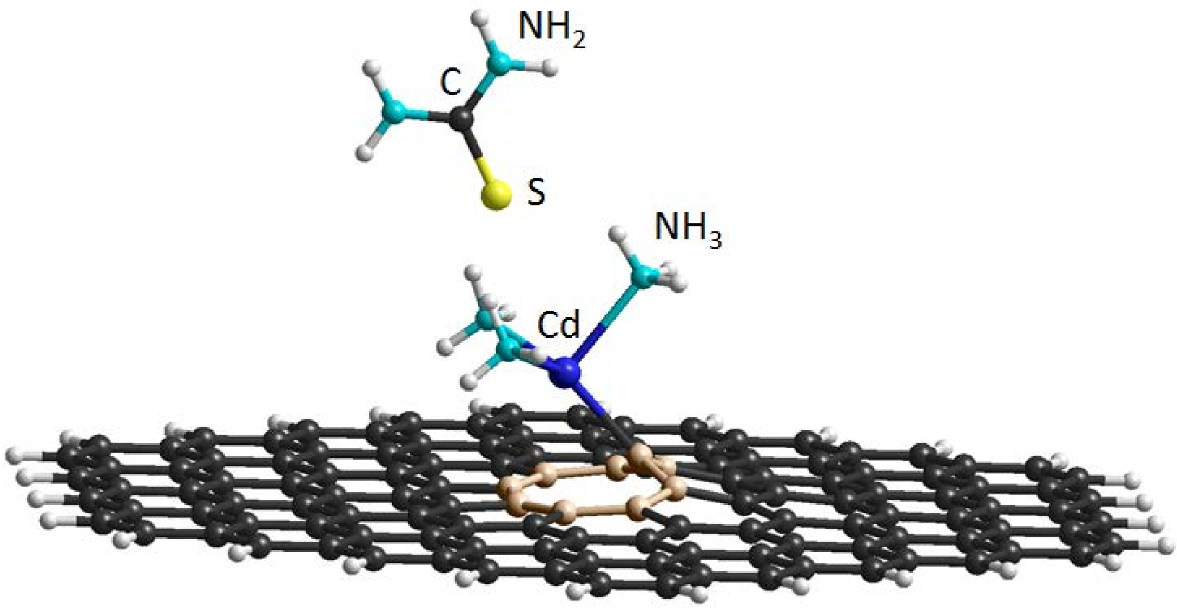

Figure S7. Leaving of $SC(NH_2)_2$ molecule of the $[Cd(NH_3)_3SC(NH_2)_2]^{2+}$ complex as the result of Cd attachment to two-fold coordinated carbon atom at the edge of monovacancy in a graphene fragment. Geometry of the model was relaxed at the B3LYP/LACVP** level. Carbon atoms constituting defects in graphene are highlighted.

Table S1. Bond lengths in free $[Cd(NH_3)_iSH]^{1+}$ complex (i=3, 2, 1, 0) and that attached to a monovacancy in graphene fragment.

Complex	**Bond length (Å)**			
	Free complex		**Attached complex**	
	Cd-S	**Cd-N**	**Cd-S**	**Cd-N**
$[Cd(NH_3)_3SH]^{1+}$	2.456	2.407; 2.421; 2.421	2.627	2.482; 2.483; 2.523
$[Cd(NH_3)_2SH]^{1+}$	2.413	2.364; 2.381	2.514	2.491; 2.497
$[Cd(NH_3)SH]^{1+}$	2.381	2.291	2.467	2.476

$[CdSH]^{1+}$	2.405	-	2.432	-

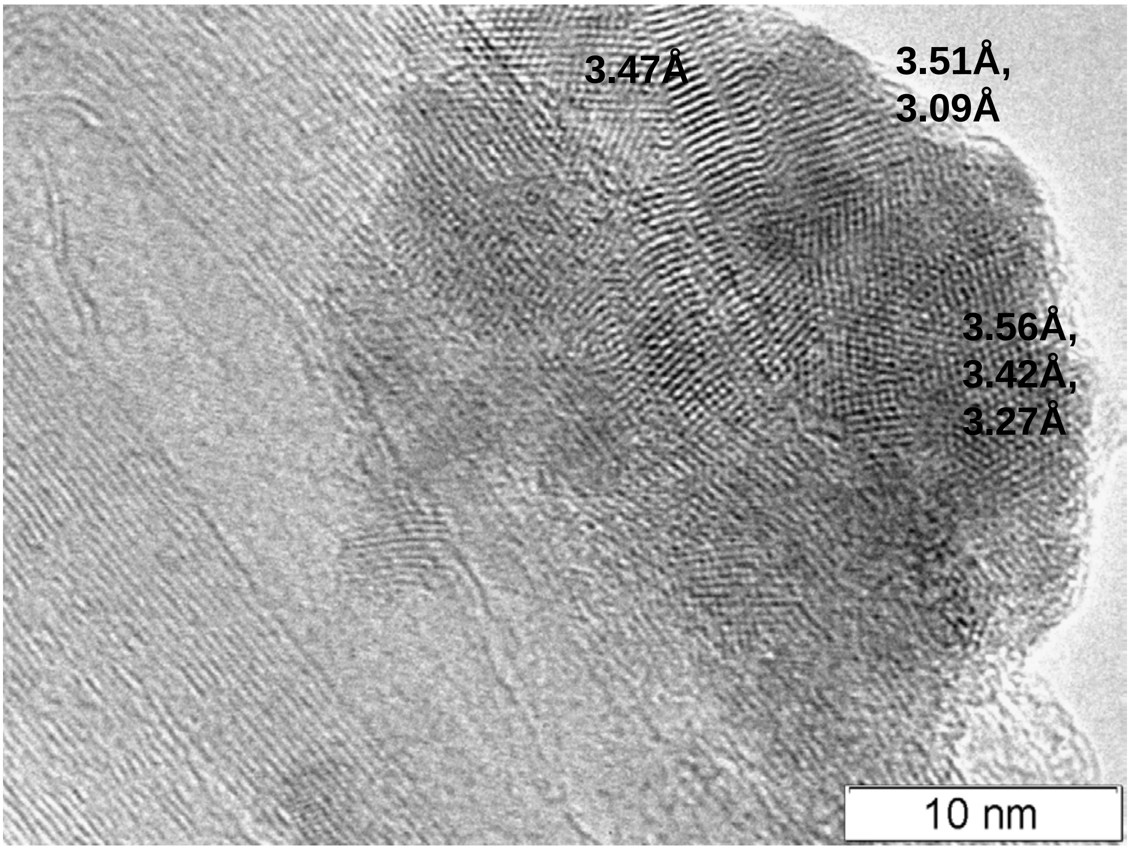

Figure S8. HRTEM image of polycrystalline CdS nanoparticle grown on the surface of the annealed MWCNTs after their 10 min immersing into chemical bath. The interlayer distances point at hexagonal lattice of nanocrystals.